

09868894

of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

FILE 'HOME' ENTERED AT 12:09:16 ON 09 OCT 2002

FILE 'REGISTRY' ENTERED AT 12:09:26 ON 09 OCT 2002
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STRUCTURE FILE UPDATES: 7 OCT 2002 HIGHEST RN 459783-15-4
DICTIONARY FILE UPDATES: 7 OCT 2002 HIGHEST RN 459783-15-4

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

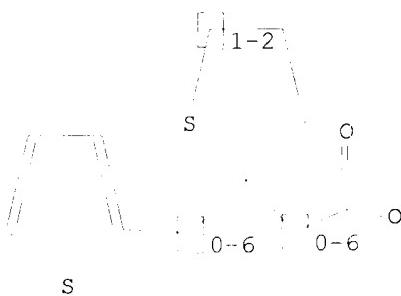
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> Uploading 09868894.str

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STE



Structure attributes must be viewed using STN Express query preparation.

09868894

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSSPTA1613SXW

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

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NEWS 4 Apr 09 ZDB will be removed from STN
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NEWS 6 Apr 20 Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS
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NEWS 8 Apr 22 Federal Research in Progress (FEDRIP) now available
NEWS 9 Jun 03 New e-mail delivery for search results now available
NEWS 10 Jun 10 MEDLINE Reload
NEWS 11 Jun 10 FCTFULL has been reloaded
NEWS 12 Jul 02 FOREGE no longer contains STANDARDS file segment
NEWS 13 Jul 22 USAN to be reloaded July 28, 2002;
 saved answer sets no longer valid
NEWS 14 Jul 29 Enhanced polymer searching in REGISTRY
NEWS 15 Jul 30 NETFIRST to be removed from STN
NEWS 16 Aug 08 CANCERLIT reload
NEWS 17 Aug 08 PHARMAMarketLetter(PHARMAML) - new on STN
NEWS 18 Aug 08 NTIS has been reloaded and enhanced
NEWS 19 Aug 19 Aquatic Toxicity Information Retrieval (AQUIRE)
 now available on STN
NEWS 20 Aug 19 IFIPAT, IFICDB, and IFIUDB have been reloaded
NEWS 21 Aug 19 The MEDLINE file segment of TOXCENTER has been reloaded
NEWS 22 Aug 26 Sequence searching in REGISTRY enhanced
NEWS 23 Sep 03 JAFIO has been reloaded and enhanced
NEWS 24 Sep 16 Experimental properties added to the REGISTRY file
NEWS 25 Sep 16 Indexing added to some pre-1967 records in CA/CAPLUS
NEWS 26 Sep 16 CA Section Thesaurus available in CAPLUS and CA
NEWS 27 Oct 01 CASREACT Enriched with Reactions from 1907 to 1985

NEWS EXPRESS February 1 CURRENT WINDOWS VERSION IS V6.0d,
 CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP),
 AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002
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=> s 11 sss sam
SAMPLE SEARCH INITIATED 12:09:49 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 82 TO ITERATE

100.0% PROCESSED 82 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1097 TO 2183
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s 11 full
FULL SEARCH INITIATED 12:09:57 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1660 TO ITERATE

100.0% PROCESSED 1660 ITERATIONS 15 ANSWERS
SEARCH TIME: 00.00.06

L3 15 SEA SSS FUL L1

=> fil caplus
COST IN U.S. DOLLARS SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 140.28 140.49

FILE 'CAPLUS' ENTERED AT 12:10:07 ON 09 OCT 2002
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FILE COVERS 1907 - 9 Oct 2002 VOL 137 ISS 15
FILE LAST UPDATED: 8 Oct 2002 (20021008/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> s 13 full
L4 1 L3

09868894

=> d 14 ibib abs hitstr

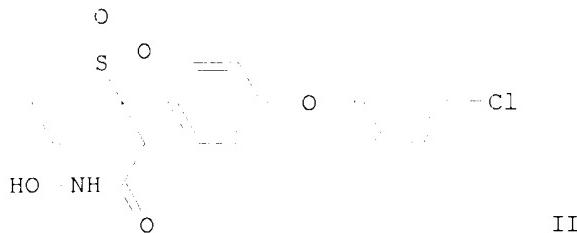
L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:475658 CAPLUS
DOCUMENT NUMBER: 133:104964
TITLE: Preparation of tetrahydro-2H-thiopyran-1,1-dioxides as
inhibitors of matrix metalloproteinases or tumor
necrosis factor .alpha.
INVENTOR(S): Taniguchi, Kiyoshi; Neya, Masahiro; Terasawa, Takeshi;
Yamazaki, Hitoshi; Sato, Kentaro; Hosoi, Kumi;
Tomishima, Yasuyo; Yoshida, Noriko; Imamura,
Yoshimasa; Takasugi, Hisashi; Setoi, Hiroyuki
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 336 pp.
CODEN: PIKXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000040576	A2	20000713	WO 2000-JP18	20000106
WO 2000040576	A3	20010322		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1140895	A2	20011010	EP 2000-900122	20000106
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 2000008589	A	20020129	BR 2000-8589	20000106
PRIORITY APPLN. INFO.:			AU 1999-8068	A 19990107
			AU 1999-1702	A 19990719
			WO 2000-JP18	W 20000106

OTHER SOURCE(S): MARPAT 133:104964
GI

A
Y Z

$R^1 - X - Ar - (CH_2)_m - (CH_2)_n - R^2 - I$



AB The title compds. (I) [wherein R^1 = alkyl, halogen, (un)substituted heterocyclic or aryl; R^2 = (protected or amidated) carboxy; Ar = (un)substituted aryl heterocyclic; A = alkylene; X = O or a single bond; Y = S, $S(O)$, or SO_2 ; Z = methylene, S, $S(O)$, or SO_2 ; m and n = independently 0-6, and $1 \leq m+n \leq 6$] and their salts were prepd. by addn. reactions of alkyl or aryl halides with tetrahydro-2H-thiopyrans and subsequent oxidn. to form the 1,1-dioxides. For example, II was synthesized in a multi-step sequence involving (1) etherification of 3,4,5,6-tetrahydro-2-(4-hydroxyphenyl)-2H-thiopyran (preparation given) with 4-bromochlorobenzene, (2) addn. of tert-Bu bromoacetate, (3) formation of the 1,1-dioxide using oxone, (4) deesterification with CF_3CO_2H , and (5) amidation of the acid with hydroxylammonium chloride. In an in vitro assay, II suppressed matrix metalloproteinase 13 (MMP-13) activity with IC_{50} of 2.2 nM. I are useful for the treatment and/or prevention of diseases such as stroke, arthritis, cancer, tissue ulceration, decubitus ulcer, restenosis, periodontal disease, epidermolysis bullosa, scleritis, psoriasis, and other disease characterized by MMP activity, as well as IADS, sepsis, septic shock, and other diseases caused by the prodn. of TNF .alpha. (no data).

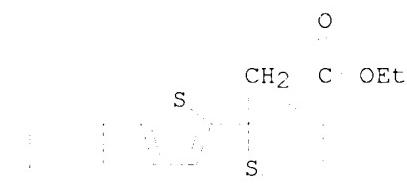
IT **282111-59-5P 282112-21-4P 282112-62-3P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of tetrahydro-2H-thiopyran 1,1-dioxides as MMP or TNF .alpha. inhibitors by addn. reactions of alkyl or aryl halides with tetrahydro-2H-thiopyrans and subsequent oxidn. to form the 1,1-dioxides)

RN 282111-59-5 CAPLUS

CN 2H-Thiopyran-2-acetic acid, 2-[5-(4-fluorophenyl)-2-thienyl]tetrahydro-, ethyl ester (9CI) (CA INDEX NAME)

F

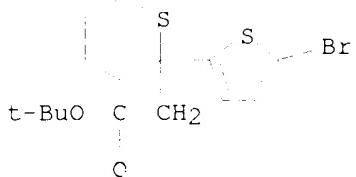


C9868894

RN 282112-21-4 CAPLUS
CN 2H-Thiopyran-2-acetic acid, 2-(5-bromo-2-thienyl)tetrahydro-, 1,1-dioxide
(9CI) (CA INDEX NAME)



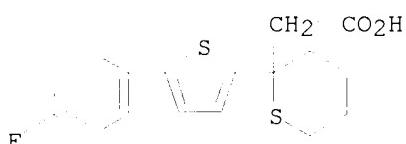
RN 282112-62-3 CAPLUS
CN 2H-Thiopyran-2-acetic acid, 2-(5-bromo-2-thienyl)tetrahydro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



IT 282111-40-4P 282111-49-3P 282111-65-3P
282111-66-4P 282112-13-4P 282112-20-3P
282115-44-0P 282115-45-1P 282115-46-2P
282115-47-3P 282533-82-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of tetrahydro-2H-thiopyran 1,1-dioxides as MMP or TNF .alpha. inhibitors by addn. reactions of alkyl or aryl halides with tetrahydro-2H-thiopyrans and subsequent oxidn. to form the 1,1-dioxides)

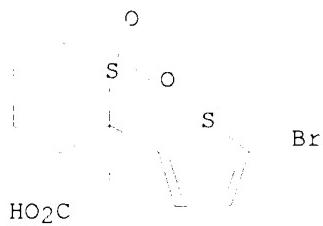
RN 282111-40-4 CAPLUS
CN 2H-Thiopyran-2-acetic acid, 2-[5-(4-fluorophenyl)-2-thienyl]tetrahydro- (9CI) (CA INDEX NAME)



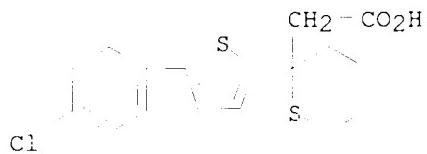
RN 282111-49-3 CAPLUS
CN 2H-Thiopyran-2-acetic acid, 2-(5-bromo-2-thienyl)tetrahydro-, 1,1-dioxide, (-) (9CI) (CA INDEX NAME)

Rotation (-).

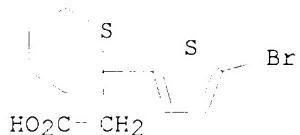
09868894



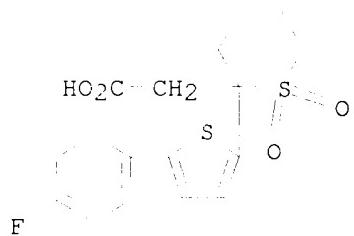
RN 282111-65-3 CAPLUS
CN 2H-Thiopyran-2-acetic acid, 2-[5-(4-chlorophenyl)-2-thienyl]tetrahydro- (9CI) (CA INDEX NAME)



RN 282111-66-4 CAPLUS
CN 2H-Thiopyran-2-acetic acid, 2-(5-bromo-2-thienyl)tetrahydro- (9CI) (CA INDEX NAME)

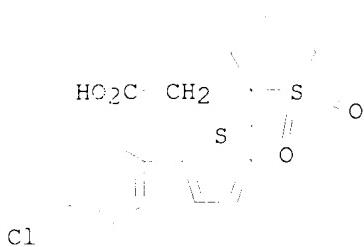


RN 282112-13-4 CAPLUS
CN 2H-Thiopyran-2-acetic acid, 2-[5-(4-fluorophenyl)-2-thienyl]tetrahydro-, 1,1-dioxide (9CI) (CA INDEX NAME)



RN 282112-20-3 CAPLUS
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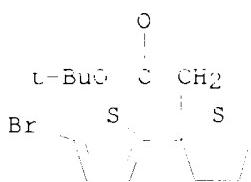
09868894



Cl

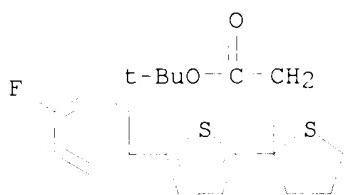
RN 282115-44-0 CAPLUS

CN [2,2'-Bithiophene]-2(3H)-acetic acid, 5'-bromo-4,5-dihydro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



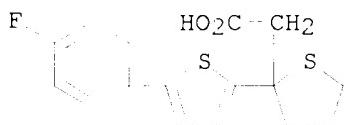
RN 282115-45-1 CAPLUS

CN [2,2'-Bithiophene]-2(3H)-acetic acid, 5'-(4-fluorophenyl)-4,5-dihydro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



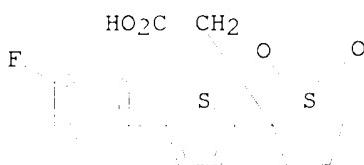
RN 282115-46-2 CAPLUS

CN [2,2'-Bithiophene]-2(3H)-acetic acid, 5'-(4-fluorophenyl)-4,5-dihydro- (9CI) (CA INDEX NAME)



RN 282115-47-3 CAPLUS

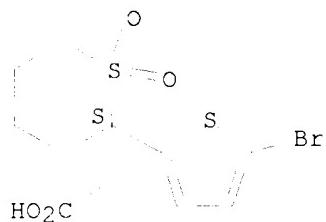
CN [2,2'-Bithiophene]-2(3H)-acetic acid, 5'-(4-fluorophenyl)-4,5-dihydro-, 1,1-dioxide (9CI) (CA INDEX NAME)



09868894

RN 282533-82-8 CAPLUS
CN 2H-Thiopyran-2-acetic acid, 2-(5-bromo-2-thienyl)tetrahydro-, 1,1-dioxide,
(2S)- (9CI) (CA INDEX NAME)

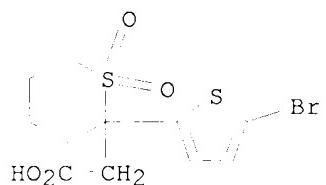
Absolute stereochemistry.



IT 282117-06-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. of tetrahydro-2H-thiopyran 1,1-dioxides as MMP or TNF .alpha.
inhibitors by addn. reactions of alkyl or aryl halides with
tetrahydro-2H-thiopyrans and subsequent oxidn. to form the
1,1-dioxides)
RN 282117-06-0 CAPLUS
CN 2H-Thiopyran-2-acetic acid, 2-(5-bromo-2-thienyl)tetrahydro-, 1,1-dioxide,
compd. with (.alpha.R)-.alpha.-methylbenzenemethanamine (1:1) (9CI) (CA
INDEX NAME)

CM 1

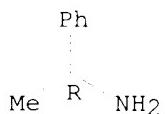
CRN 282112-21-4
CMF C11 H13 Br O4 S2



CM 2

CRN 3886-69-9
CMF C8 H11 N

Absolute stereochemistry.



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PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

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| NEWS | 3 | Apr 09 BEILSTEIN: Reload and Implementation of a New Subject Area |
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| NEWS | 10 | Jun 10 MEDLINE Reload |
| NEWS | 11 | Jun 10 PCTFULL has been reloaded |
| NEWS | 12 | Jul 02 FOREGE no longer contains STANDARDS file segment |
| NEWS | 13 | Jul 22 USAN to be reloaded July 28, 2002;
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| NEWS | 14 | Jul 29 Enhanced polymer searching in REGISTRY |
| NEWS | 15 | Jul 30 NETFIRST to be removed from STN |
| NEWS | 16 | Aug 08 CANCERLIT reload |
| NEWS | 17 | Aug 08 PHARMAMarketLetter(PHARMAML) - new on STN |
| NEWS | 18 | Aug 08 NTIS has been reloaded and enhanced |
| NEWS | 19 | Aug 19 Aquatic Toxicity Information Retrieval (AQUIRE)
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| NEWS | 23 | Sep 03 JAPIO has been reloaded and enhanced |
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| NEWS | 26 | Sep 16 CA Section Thesaurus available in CAPLUS and CA |
| NEWS | 27 | Oct 01 CASREACT Enriched with Reactions from 1907 to 1985 |
| NEWS EXPRESS | | February 1 CURRENT WINDOWS VERSION IS V6.0d,
CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP),
AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002 |
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FILE 'REGISTRY' ENTERED AT 12:20:30 ON 09 OCT 2002
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STRUCTURE FILE UPDATES: 7 OCT 2002 HIGHEST RN 459783-15-4
DICTIONARY FILE UPDATES: 7 OCT 2002 HIGHEST RN 459783-15-4

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

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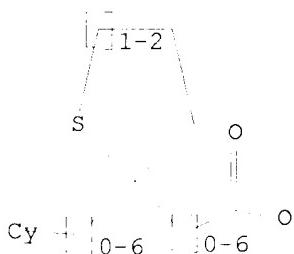
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>
Uploading 09868894b.str

STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

09868894

=> s 11 sss sam
SAMPLE SEARCH INITIATED 12:20:46 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 921 TO ITERATE

100.0% PROCESSED 921 ITERATIONS 4 ANSWERS
SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 16600 TO 20240
PROJECTED ANSWERS: 4 TO 200

L2 4 SEA SSS SAM L1

=> s 11 full
FULL SEARCH INITIATED 12:20:53 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 19418 TO ITERATE

100.0% PROCESSED 19418 ITERATIONS 73 ANSWERS
SEARCH TIME: 00.00.04

L3 73 SEA SSS FUL L1

=> fil cap;us
COST IN U.S. DOLLARS SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 140.28 140.49

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FILE COVERS 1907 - 9 Oct 2002 VOL 137 ISS 15
FILE LAST UPDATED: 8 Oct 2002 (20021008/ED)

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US IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter

09868894

"HELP COMMANDS" at an arrow prompt (=>).

| | | |
|----------------------|------------|---------|
| => fil caplus | SINCE FILE | TOTAL |
| COST IN U.S. DOLLARS | ENTRY | SESSION |
| FULL ESTIMATED COST | 0.40 | 140.89 |

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FILE COVERS 1907 - 9 Oct 2002 VOL 137 ISS 15
FILE LAST UPDATED: 8 Oct 2002 (20021008/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

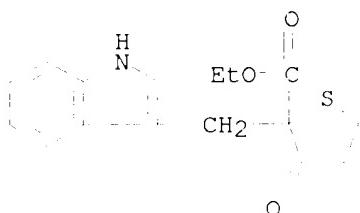
=> s 13 full
L4 17 L3

=> d 14 1-17 ibib abs hitstr

L4 ANSWER 1 OF 17 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2001:481440 CAPLUS
DOCUMENT NUMBER: 135:210899
TITLE: The Use of Sulfur Ylides in the Synthesis of Substituted Indoles
AUTHOR(S): Kennedy, Abigail R.; Taday, Michael H.; Rainier, Jon D.
CORPORATE SOURCE: Department of Chemistry, The University of Arizona, Tucson, AZ, 85721, USA
SOURCE: Organic Letters (2001), 3(15), 2407-2409
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB C-10 thioindoles (3-ethylthiomethylindoles) undergo fragmentation-coupling reactions when exposed to rhodium carbenoids. In an analogous fashion, keto ester- and malonate-substituted carbenoids insert into indole C-2 thioethers. In contrast, vinylogous carbenoids alkylate indole C-2 thioethers at C-3.
IT 357981-89-6P
RL: SPN (Synthetic preparation); PREP (Preparation)

09868894

(substitution reactions of indole thioethers via sulfur ylides)
RN 357981-89-6 CAPLUS
CN 2-Thiophenecarboxylic acid, tetrahydro-2-(1H-indol-3-ylmethyl)-3-oxo-,
ethyl ester (9CI) (CA INDEX NAME)



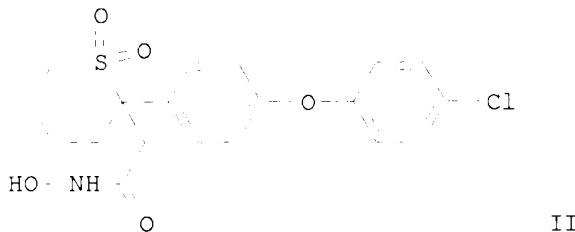
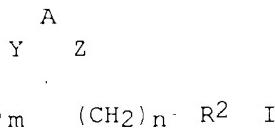
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 17 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:475658 CAPLUS
DOCUMENT NUMBER: 133:104964
TITLE: Preparation of tetrahydro-2H-thiopyran-1,1-dioxides as inhibitors of matrix metalloproteinases or tumor necrosis factor .alpha.
INVENTOR(S): Taniguchi, Kiyoshi; Neya, Masahiro; Terasawa, Takeshi; Yamazaki, Hitoshi; Sato, Kentaro; Hosoi, Kumi; Tomishima, Yasuyo; Yoshida, Noriko; Imamura, Yoshimasa; Takasugi, Hisashi; Setoi, Hiroyuki
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 336 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|-----------------|------------|
| WO 2000040576 | A2 | 20000713 | WO 2000-JP18 | 20000106 |
| WO 2000040576 | A3 | 20010322 | | |
| W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ,
DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS,
JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN,
MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM,
TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD,
RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| EP 1140895 | A2 | 20011010 | EP 2000-900122 | 20000106 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO | | | | |
| BR 2000008589 | A | 20020129 | BR 2000-8589 | 20000106 |
| PRIORITY APPLN. INFO.: | | | AU 1999-8068 | A 19990107 |
| | | | AU 1999-1702 | A 19990719 |
| | | | WO 2000-JP18 | W 20000106 |

OTHER SOURCE(S): MARPAT 133:104964

GI



AB The title compds. (I) [wherein R₁ = alkyl, halogen, (un)substituted heterocyclic or aryl; R₂ = (protected or amidated) carboxy; Ar = (un)substituted aryl heterocyclic; A = alkylene; X = O or a single bond; Y = S, S(O), or SO₂; Z = methylene, S, S(O), or SO₂; m and n = independently 0-6, and 1 .ltoreq. m+n .ltoreq. 6] and their salts were prep'd. by addn. reactions of alkyl or aryl halides with tetrahydro-2H-thiopyrans and subsequent oxidn. to form the 1,1-dioxides. For example, II was synthesized in a multi-step sequence involving (1) etherification of 3,4,5,6-tetrahydro-2-(4-hydroxyphenyl)-2H-thiopyran (preparation given) with 4-bromochlorobenzene, (2) addn. of tert-Bu bromoacetate, (3) formation of the 1,1-dioxide using oxone, (4) deesterification with CF₃CO₂H, and (5) amidation of the acid with hydroxylammonium chloride. In an in vitro assay, II suppressed matrix metalloproteinase 13 (MMP-13) activity with IC₅₀ of 2.2 nM. I are useful for the treatment and/or prevention of diseases such as stroke, arthritis, cancer, tissue ulceration, decubitus ulcer, restenosis, periodontal disease, epidermolysis bullosa, scleritis, psoriasis, and other disease characterized by MMP activity, as well as IADS, sepsis, septic shock, and other diseases caused by the prodn. of TNF .alpha. (no data).

IT 282111-38-0P 282111-44-8P 282111-45-9P
 282111-46-0P 282111-48-2P 282111-59-5P
 282111-61-9P 282112-11-2P 282112-21-4P
 282112-23-6P 282112-26-9P 282112-62-3P

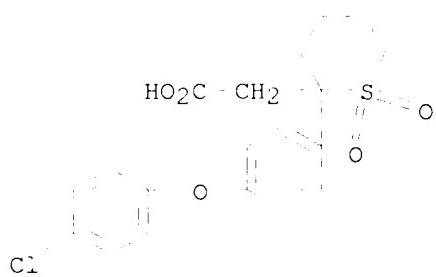
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of tetrahydro-2H-thiopyran 1,1-dioxides as MMP or TNF .alpha. inhibitors by addn. reactions of alkyl or aryl halides with tetrahydro-2H-thiopyrans and subsequent oxidn. to form the 1,1-dioxides)

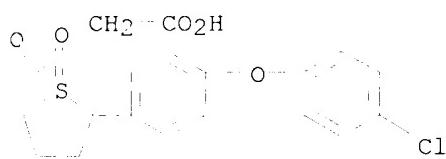
RN 282111-38-0 CAPLUS

CN 2H-Thiopyran-2-acetic acid, 2-[4-(4-chlorophenoxy)phenyl]tetrahydro-, 1,1-dioxide (9CI) (CA INDEX NAME)

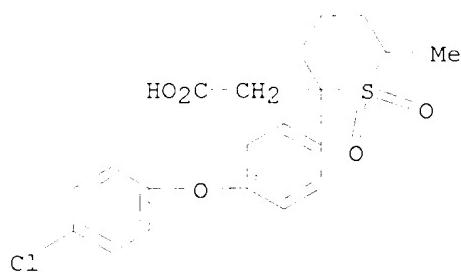
09868894



RN 282111-44-8 CAPLUS
CN 2H-Thiopheneacetic acid, 2-[4-(4-chlorophenoxy)phenyl]tetrahydro-,
1,1-dioxide (9CI) (CA INDEX NAME)

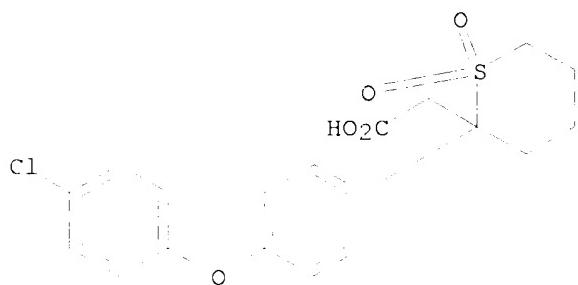


RN 282111-45-9 CAPLUS
CN 2H-Thiopyran-2-acetic acid, 2-[4-(4-chlorophenoxy)phenyl]tetrahydro-6-
methyl-, 1,1-dioxide (9CI) (CA INDEX NAME)



RN 282111-46-0 CAPLUS
CN 2H-Thiopyran-2-acetic acid, 2-[4-(4-chlorophenoxy)phenyl]tetrahydro-,
1,1-dioxide, (-)- (9CI) (CA INDEX NAME)

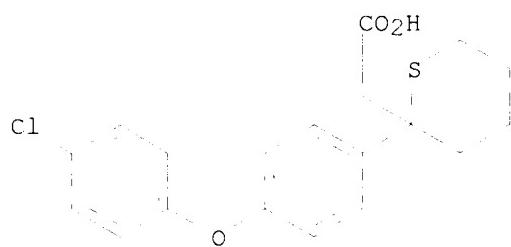
Rotation (-).



RN 282111-48-2 CAPLUS
CN 2H-Thiopyran-2-acetic acid, 2-[4-(4-chlorophenoxy)phenyl]tetrahydro-, (-)-
(9CI) (CA INDEX NAME)

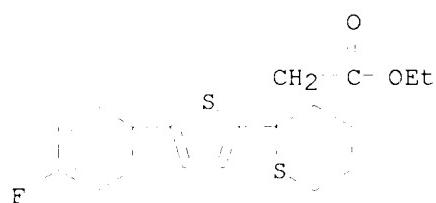
09868894

Rotation (-).



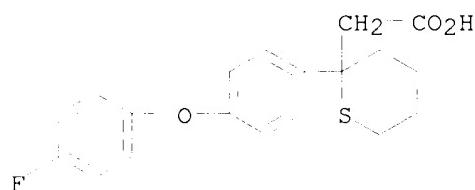
RN 282111-59-5 CAPLUS

CN 2H-Thiopyran-2-acetic acid, 2-[5-(4-fluorophenyl)-2-thienyl]tetrahydro-, ethyl ester (9CI) (CA INDEX NAME)



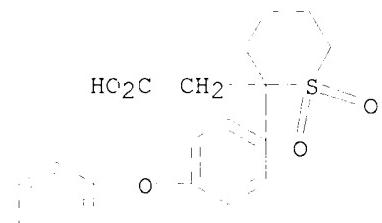
RN 282111-61-9 CAPLUS

CN 2H-Thiopyran-2-acetic acid, 2-[4-(4-fluorophenoxy)phenyl]tetrahydro- (9CI) (CA INDEX NAME)



RN 282112-11-2 CAPLUS

CN 2H-Thiopyran-2-acetic acid, 2-[4-(4-bromophenoxy)phenyl]tetrahydro-, 1,1-dioxide (9CI) (CA INDEX NAME)



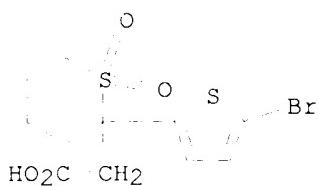
Br

RN 282112-21-4 CAPLUS

CN 2H-Thiopyran-2-acetic acid, 2-(5-bromo-2-thienyl)tetrahydro-, 1,1-dioxide

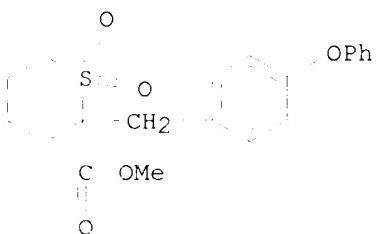
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(9CI) (CA INDEX NAME)



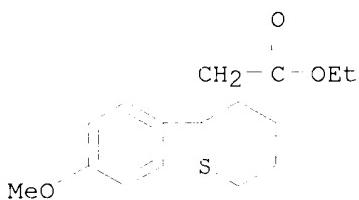
RN 282112-23-6 CAPLUS

CN 2H-Thiopyran-2-carboxylic acid, tetrahydro-2-[(4-phenoxyphenyl)methyl]-, methyl ester, 1,1-dioxide (9CI) (CA INDEX NAME)



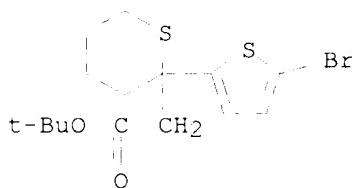
RN 282112-26-9 CAPLUS

CN 2H-Thiopyran-2-acetic acid, tetrahydro-2-(4-methoxyphenyl)-, ethyl ester (9CI) (CA INDEX NAME)



RN 282112-62-3 CAPLUS

CN 2H-Thiopyran-2-acetic acid, 2-(5-bromo-2-thienyl)tetrahydro-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



IT 282111-39-1P 282111-40-4P 282111-41-5P

282111-42-6P 282111-47-1P 282111-49-3P

282111-50-6P 282111-57-3P 282111-58-4P

282111-60-8P 282111-62-0P 282111-63-1P

282111-64-2P 282111-65-3P 282111-66-4P

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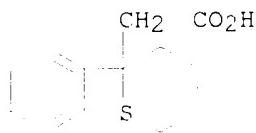
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282112-14-5P 282112-15-6P 282112-16-7P
282112-17-8P 282112-19-0P 282112-20-3P
282112-22-5P 282112-24-7P 282112-25-8P
282115-44-0P 282115-45-1P 282115-46-2P
282115-47-3P 282533-82-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prep. of tetrahydro-2H-thiopyran 1,1-dioxides as MMP or TNF .alpha. inhibitors by addn. reactions of alkyl or aryl halides with tetrahydro-2H-thiopyrans and subsequent oxidn. to form the 1,1-dioxides)

RN 282111-39-1 CAPLUS

CN 2H-Thiopyran-2-acetic acid, tetrahydro-2-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

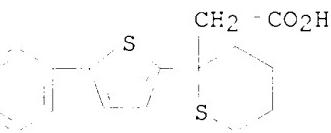
MeO



RN 282111-40-4 CAPLUS

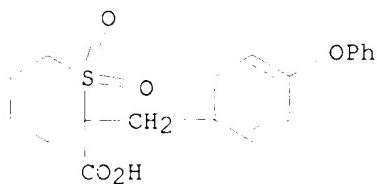
CN 2H-Thiopyran-2-acetic acid, 2-[5-(4-fluorophenyl)-2-thienyl]tetrahydro- (9CI) (CA INDEX NAME)

F



RN 282111-41-5 CAPLUS

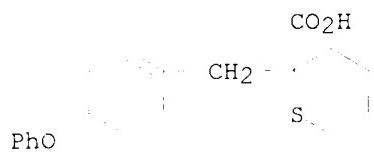
CN 2H-Thiopyran-2-carboxylic acid, tetrahydro-2-[(4-phenoxyphenyl)methyl]-, 1,1-dioxide (9CI) (CA INDEX NAME)



RN 282111-42-6 CAPLUS

CN 2H-Thiopyran-2-carboxylic acid, tetrahydro-2-[(4-phenoxyphenyl)methyl]- (9CI) (CA INDEX NAME)

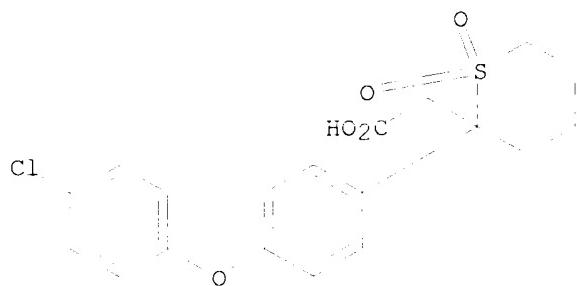
09868894



RN 282111-47-1 CAPLUS

CN 2H-Thiopyran-2-acetic acid, 2-[4-(4-chlorophenoxy)phenyl]tetrahydro-, 1,1-dioxide, (+)- (9CI) (CA INDEX NAME)

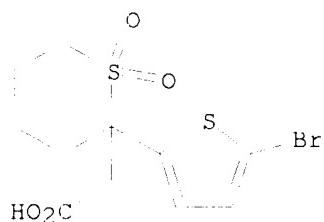
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RN 282111-49-3 CAPLUS

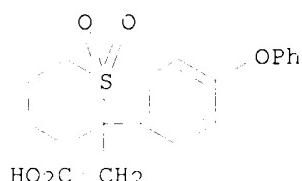
CN 2H-Thiopyran-2-acetic acid, 2-(5-bromo-2-thienyl)tetrahydro-, 1,1-dioxide, (-)- (9CI) (CA INDEX NAME)

Rotation (-).



RN 282111-50-6 CAPLUS

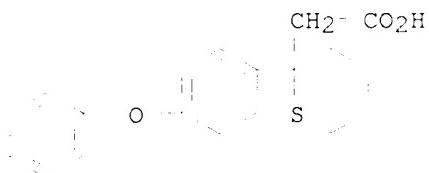
CN 2H-Thiopyran-2-acetic acid, tetrahydro-2-(4-phenoxyphenyl)-, 1,1-dioxide (9CI) (CA INDEX NAME)



RN 282111-57-3 CAPLUS

CN 2H-Thiopyran-2-acetic acid, 2-[4-(4-chlorophenoxy)phenyl]tetrahydro- (9CI) (CA INDEX NAME)

09868894



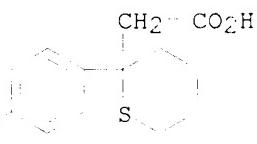
Cl

RN 282111-58-4 CAPLUS
CN 2H-Thiopyran-2-acetic acid, 2-[4-(4-bromophenoxy)phenyl]tetrahydro- (9CI)
(CA INDEX NAME)



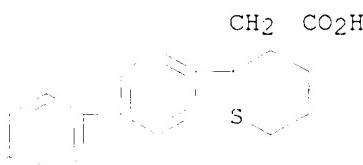
Br

RN 282111-60-8 CAPLUS
CN 2H-Thiopyran-2-acetic acid, 2-[1,1'-biphenyl]-4-yltetrahydro- (9CI) (CA INDEX NAME)



Ph

RN 282111-62-0 CAPLUS
CN 2H-Thiopyran-2-acetic acid, 2-(4'-chloro[1,1'-biphenyl]-4-yl)tetrahydro- (9CI) (CA INDEX NAME)



Cl

RN 282111-63-1 CAPLUS
CN 2H-Thiopyran-2-acetic acid, 2-(4'-bromo[1,1'-biphenyl]-4-yl)tetrahydro- (9CI) (CA INDEX NAME)

09868894

CH₂ CO₂H



Br

RN 282111-64-2 CAPLUS

CN 2H-Thiopyran-2-acetic acid, 2-(4'-fluoro[1,1'-biphenyl]-4-yl)tetrahydro- (9CI) (CA INDEX NAME)

CH₂ CO₂H



F

RN 282111-65-3 CAPLUS

CN 2H-Thiopyran-2-acetic acid, 2-[5-(4-chlorophenyl)-2-thienyl]tetrahydro- (9CI) (CA INDEX NAME)

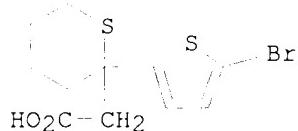
CH₂ CO₂H



Cl

RN 282111-66-4 CAPLUS

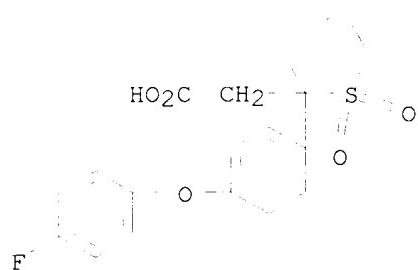
CN 2H-Thiopyran-2-acetic acid, 2-(5-bromo-2-thienyl)tetrahydro- (9CI) (CA INDEX NAME)



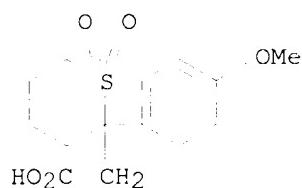
RN 282112-10-1 CAPLUS

CN 2H-Thiopyran-2-acetic acid, 2-[4-(4-fluorophenoxy)phenyl]tetrahydro-, 1,1-dioxide (9CI) (CA INDEX NAME)

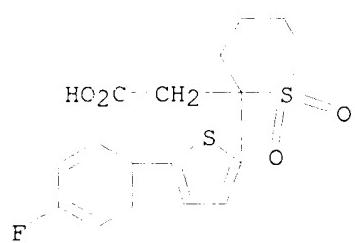
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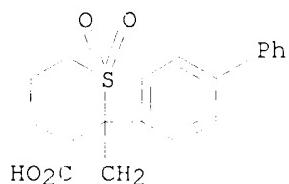
RN 282112-12-3 CAPLUS
CN 2H-Thiopyran-2-acetic acid, tetrahydro-2-(4-methoxyphenyl)-, 1,1-dioxide
(9CI) (CA INDEX NAME)



RN 282112-13-4 CAPLUS
CN 2H-Thiopyran-2-acetic acid, 2-[5-(4-fluorophenyl)-2-thienyl]tetrahydro-,
1,1-dioxide (9CI) (CA INDEX NAME)

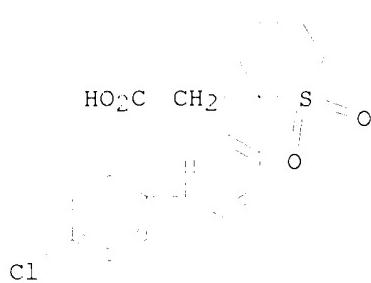


RN 282112-14-5 CAPLUS
CN 2H-Thiopyran-2-acetic acid, 2-[1,1'-biphenyl]-4-yltetrahydro-, 1,1-dioxide
(9CI) (CA INDEX NAME)

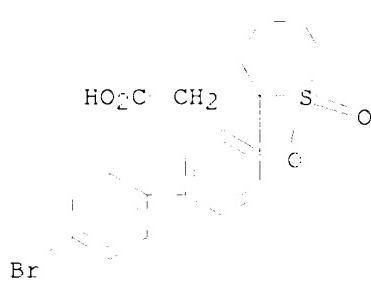


RN 282112-15-6 CAPLUS
CN 2H-Thiopyran-2-acetic acid, 2-(4'-chloro[1,1'-biphenyl]-4-yl)tetrahydro-,
1,1-dioxide (9CI) (CA INDEX NAME)

09868894

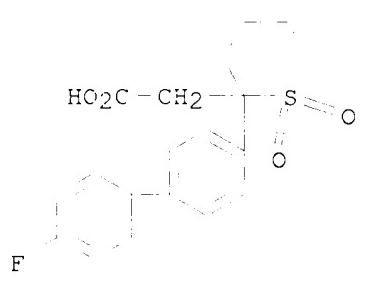


RN 282112-16-7 CAPLUS
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1,1-dioxide (9CI) (CA INDEX NAME)



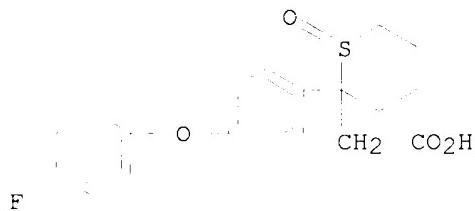
Br

RN 282112-17-8 CAPLUS
CN 2H-Thiopyran-2-acetic acid, 2-(4'-fluorobiphenyl)-4-yl tetrahydro-,
1,1-dioxide (9CI) (CA INDEX NAME)



F

RN 282112-19-0 CAPLUS
CN 2H-Thiopyran-2-acetic acid, 2-[4-(4-fluorophenoxy)phenyl]tetrahydro-,
1-oxide (9CI) (CA INDEX NAME)



F

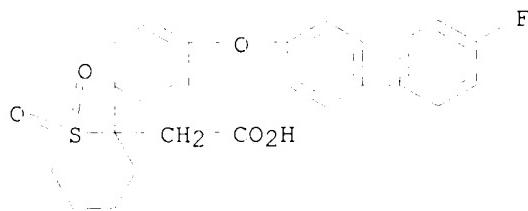
RN 282112-20-3 CAPLUS
CN 2H-Thiopyran-2-acetic acid, 2-[5-(4-chlorophenyl)-2-thienyl]tetrahydro-,

09868894

1,1-dioxide (9CI) (CA INDEX NAME)

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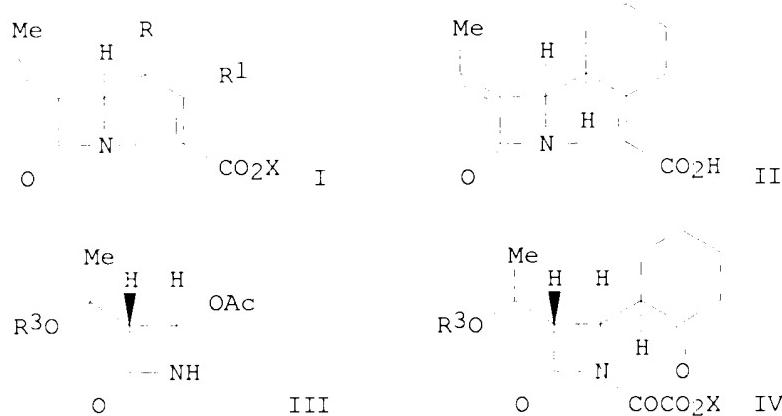
RN 282112-22-5 CAPLUS
CN 2H-Thiopyran-2-acetic acid, 2-[4-[(4'-fluoro[1,1'-biphenyl]-4-yl)oxy]phenyl]tetrahydro-, 1,1-dioxide (9CI) (CA INDEX NAME)



=> d 14 3-17 ibib abs hitstr

L4 ANSWER 3 OF 17 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:424253 CAPLUS
DOCUMENT NUMBER: 129:95355
TITLE: Preparation of ethylenedene derivatives of tricyclic carbapenems for use as antibiotics
INVENTOR(S): Copar, Anton; Solmajer, Tomaz; Anzic, Borut; Kuzman, Tadeja; Mesar, Tomaz; Kocjan, Darko
PATENT ASSIGNEE(S): Lek Tovarna Farmacevtskih In Kemicnih Izdelkov, Slovenia; Copar, Anton; Solmajer, Tomaz; Anzic, Borut; Kuzman, Tadeja; Mesar, Tomaz; Kocjan, Darko
SOURCE: PCT Int. Appl., 68 pp.
CODEN: PIKXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|--------|-----------|-----------------|------------|
| WO 9827094 | A1 | 19980625 | WO 1997-SI35 | 19971218 |
| W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | | |
| AU 9852375 | A1 | 19980715 | AU 1998-52375 | 19971218 |
| EP 946558 | A1 | 19991006 | EP 1997-947251 | 19971218 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI | | | | |
| JP 2001506258 | T2 | 20010515 | JP 1998-527639 | 19971218 |
| PRIORITY APPLN. INFO.: | | | SI 1996-371 | A 19961218 |
| | | | WO 1997-SI35 | W 19971218 |
| OTHER SOURCE(S): | MARPAT | 129:95355 | | |
| GI | | | | |



AB Tricyclic carbapenems I [RR1 = fused alicyclic or heterocyclic ring; X = H, alkyl, alkali metal, ammonium] were prep'd. and pharmaceutical formulations were described for use as inhibitors of the action of the enzyme .beta.-lactamase and as antibiotics in human and veterinary medicine. Thus, carbapenem II was prep'd. starting from Azetidon III (R3 = SiMe₂CMe₃) via the formation and intramol. cyclization of ester IV (R3 = SiMe₂CMe₃, X = allyl). The prep'd. compds. were tested for .beta.-lactamase inhibitory activity.

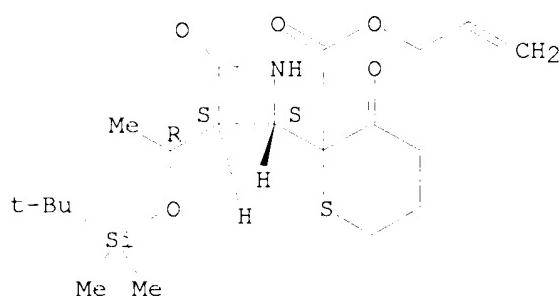
IT 209536-83-4P 209536-84-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of ethyldene derivs. of tricyclic carbapenems for use as antibiotics)

RN 209536-83-4 CAPLUS

CN 2H-Thiopyran-2-carboxylic acid, 2-[(2S,3S)-3-[(1R)-1-[(1,1-dimethylethyl)dimethylsilyl]oxy]ethyl]-4-oxo-2-azetidinyl]tetrahydro-3-oxo-, 2-propenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

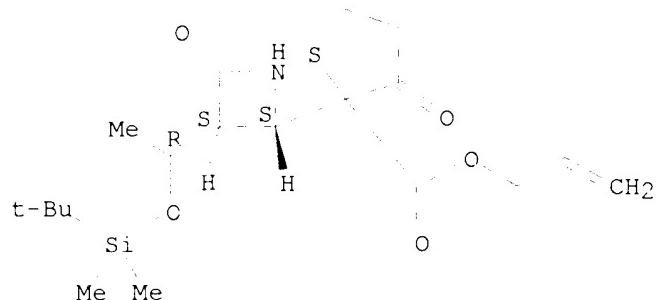


RN 209536-84-5 CAPLUS

CN 2-Thiophenecarboxylic acid, 2-[(2S,3S)-3-[(1R)-1-[(1,1-dimethylethyl)dimethylsilyl]oxy]ethyl]-4-oxo-2-azetidinyl]tetrahydro-3-oxo-, 2-propenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

09868894



L4 ANSWER 4 OF 17 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1997:638719 CAPLUS

DOCUMENT NUMBER: 127:307323

TITLE: Selective anodic monofluorination of sulfur-containing heterocycles: potent applications towards pharmaceuticals

AUTHOR(S): Fuchigami, Toshio

CORPORATE SOURCE: Dep. Electronic Chem., Tokyo Inst. Tech., Yokohama, 226, Japan

SOURCE: Phosphorus, Sulfur and Silicon and the Related Elements (1997), 120 & 121, 343-344

CODEN: PSSLEC; ISSN: 1042-6507

PUBLISHER: Gordon & Breach

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A symposium report with 3 refs. Regioselective anodic monofluorination of 3-thiolanones, 1,3-oxathiolanones, and 1,3-dithiolanones was successfully carried out in MeCN contg. Et₂N·3HF or Et₄NF·4HF as a supporting electrolyte. Among the fluorinated products, 2-benzyl-4,4-dimethyl-2-ethoxycarbonyl-5-fluoro-3-thiolanone has comparable or even stronger *in vitro* human type II phospholipase A2 inhibitory activity than manoalide.

IT 169890-90-8P

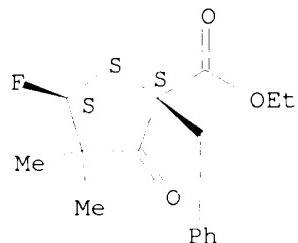
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. and human type II phospholipase A2 inhibitory activity of)

RN 169890-90-8 CAPLUS

CN 2-Thiophenecarboxylic acid, 5-fluorotetrahydro-4,4-dimethyl-3-oxo-2-(phenylmethyl)-, ethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



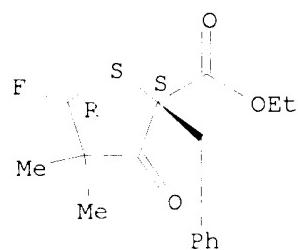
L4 ANSWER 5 OF 17 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1995:666577 CAPLUS

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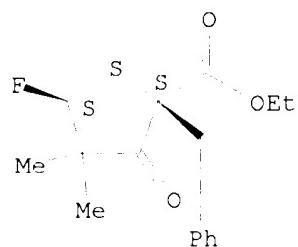
DOCUMENT NUMBER: 123:313666
TITLE: Electrolytic partial fluorination of organic compounds. 18. Electrosynthesis of 4,4-dimethyl-2-ethoxycarbonyl-5-fluoro-3-thiolanones: highly potent human type II PLA₂ inhibitors
AUTHOR(S): Narizuka, Satoru; Fuchigami, Toshio
CORPORATE SOURCE: Dep. Electronic Chem., Tokyo Inst. Technol., Yokohama, 226, Japan
SOURCE: Bioorganic & Medicinal Chemistry Letters (1995), 5(12), 1293-4
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:313666
AB Anodic monofluorination of 2-methyl- and 2-benzyl-4,4-dimethyl-2-ethoxycarbonyl-3-thiolanones was successfully performed to provide the corresponding 5-fluorinated products in good yields. The stereoisomeric mixt. of the fluorinated 2-benzyl compds. was found to possess comparable or even stronger *in vitro* human type II phospholipase A₂ inhibitory activity compared with the known inhibitor, manoolide; the *cis* isomer exhibited higher activity than the *trans* isomer.
IT 169890-89-5P 169890-90-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(electrosynthesis of dimethyl(ethoxycarbonyl)fluorothiolanones as human type II PLA₂ inhibitors)
RN 169890-89-5 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-fluorotetrahydro-4,4-dimethyl-3-oxo-2-(phenylmethyl)-, ethyl ester, *cis*- (9CI) (CA INDEX NAME)

Relative stereochemistry.

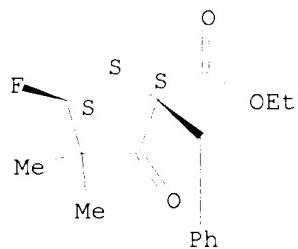


RN 169890-90-8 CAPLUS
CN 2-Thiophenecarboxylic acid, 5-fluorotetrahydro-4,4-dimethyl-3-oxo-2-(phenylmethyl)-, ethyl ester, *trans*- (9CI) (CA INDEX NAME)

Relative stereochemistry.



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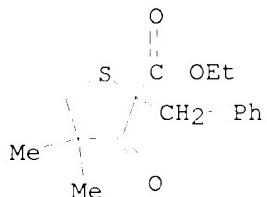


IT 169890-87-3

RL: RCT (Reactant); RACT (Reactant or reagent)
(electrosynthesis of dimethyl(ethoxycarbonyl)fluorothiolanones as human
type II PLA₂ inhibitors)

RN 169890-87-3 CAPLUS

CN 2-Thiophenecarboxylic acid, tetrahydro-4,4-dimethyl-3-oxo-2-(phenylmethyl)-,
, ethyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 6 OF 17 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1993:254446 CAPLUS

DOCUMENT NUMBER: 118:254446

TITLE: Carbocyclic and heterocyclic HIV protease inhibitors

INVENTOR(S): Chenera, Balan; Des Jarlais, Renee Louise; Dreyer, Geoffrey Bainbridge

PATENT ASSIGNEE(S): Smithkline Beecham Corp., USA

SOURCE: PCT Int. Appl., 42 pp.

CODEN: PIXXD2

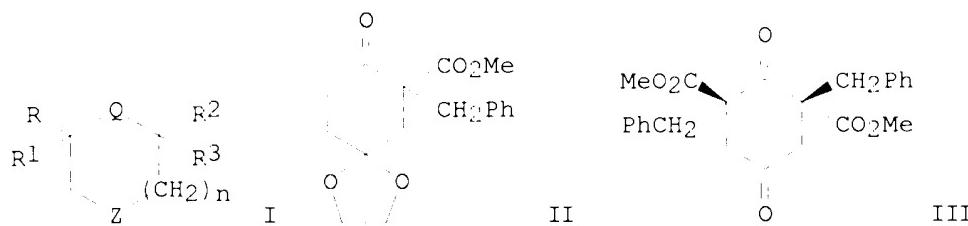
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|--------|------------|-----------------|----------|
| WO 9221647 | A1 | 19921210 | WO 1992-US4705 | 19920604 |
| W: JP, US | | | | |
| RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE | | | | |
| JP 06508146 | T2 | 19940914 | JP 1992-500653 | 19920604 |
| EP 641306 | A1 | 19950308 | EP 1992-914474 | 19920604 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, SE | | | | |
| PRIORITY APPLN. INFO.: | | | US 1991-710734 | 19910604 |
| | | | WO 1992-US4705 | 19920604 |
| OTHER SOURCE(S): | MARPAT | 118:254446 | | |
| GI | | | | |



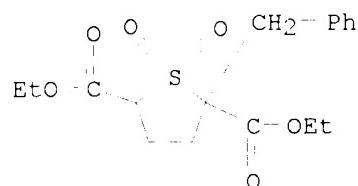
AB The heterocyclic and carbocyclic compds. I [R, R3 = HO, (CHR4)mCOR5, (CHR4)mCH(OH)R4, R4; R1, R2 = H, Cl-8-alkyl, Het, C3-10-cycloalkyl, Het-Cl-8-alkyl, C2-8-alkenyl, Het-C2-8-alkenyl, C3-10-cycloalkyl-Cl-8-alkyl, C3-10-cycloalkyl-C2-8-alkenyl; R4 = R1 or substituted R1; R5 = H, HO, alkoxy, R1, amino, etc.; Z = CH2, CHO, aminomethylene, S, SO, SO2, SONH, O, CO, substituted imino, etc.; Q = CHO, S, SO, SO2; m = 0, 1, 2; n = 0, 1] and pharmaceutical acceptable salts were prep'd. as HIV protease inhibitors and are useful in treatment of aids. Thus, 4,4-ethylenedioxycyclohexanone nucleophilic underwent addn. with NCCO2Me followed by benzylation with PhCH2Br to give cyclohexanone II, which was similarly carboxylated and benzylated followed by hydrolysis to give the cyclohexanedione III.

IT **147838-72-0P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and benzylation of)

RN 147838-72-0 CAPLUS

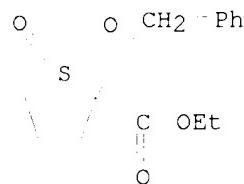
CN Hexanic acid, 2,3,4,5-tetradeoxy-2,5-episulfonyl-2-C-(phenylmethyl)-, diethyl ester (9CI) (CA INDEX NAME)

IT **147838-71-9P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and ethoxycarbonylation of)

RN 147838-71-9 CAPLUS

CN 2-Thiophenecarboxylic acid, tetrahydro-2-(phenylmethyl)-, ethyl ester, 1,1-dioxide (9CI) (CA INDEX NAME)

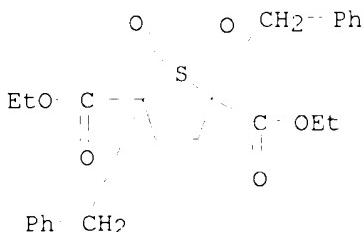
IT **147838-73-1P**

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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(prepn. and redn. of)

FN 147838-73-1 CAPLUS

CN Hexaric acid, 2,3,4,5-tetradeoxy-2,5-episulfonyl-2,5-bis-C-(phenylmethyl)-
, diethyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 7 OF 17 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1993:124354 CAPLUS

DOCUMENT NUMBER: 118:124354

TITLE: A hetero Diels-Alder approach to novel thiopyran analogs of aprikalim, a potassium channel activator

Pinto, Ivan L.; Buckle, Derek R.; Rami, Harshad K.; Smith, David G.

CORPORATE SOURCE: SmithKline Beecham Pharm., Epsom/Surrey, KT18 5XQ, UK

SOURCE: Tetrahedron Letters (1992), 33(49), 7597-600

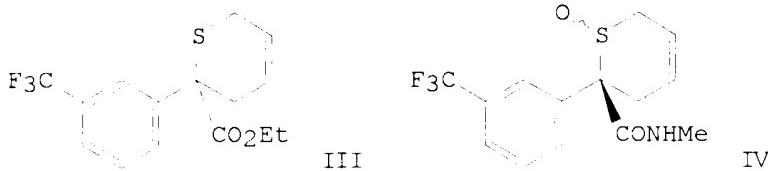
CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 118:124354

GI



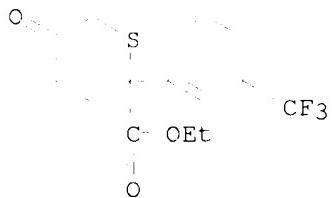
AB .alpha.-Thioketo ester 3-F3CC6H4C(S)CO2Et (I), derived from Bunte salt 2-F3CC6H4C(SSO3Na)CO2Et (II), has been shown to undergo a hetero Diels-Alder reaction with a variety of dienes to form the basis of a concise synthesis of dihydrothiopyran analogs of the potassium channel activator aprikalim. Thus, reacting II with NEt3/CaCl2/EtOH generated I which reacted with H2C:CHCH:CH2 to give thiopyran deriv. III which was converted in 4 steps to aprikalim analogs IV.

IT 146138-09-2P

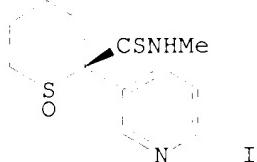
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

FN 146138-09-2 CAPLUS

CN 2H-Thiopyran-2-carboxylic acid, tetrahydro-5-oxo-2-[3-(trifluoromethyl)phenyl]-, ethyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 8 OF 17 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1992:591643 CAPLUS
 DOCUMENT NUMBER: 117:191643
 TITLE: Synthesis and biological activity of trans-(.+-.)-N-methyl-2-(3-pyridyl)-2-tetrahydrothiopyrancarbothioamide 1-oxide (RP 49356) and analogs: a new class of potassium channel opener
 Brown, Thomas J.; Chapman, Robert F.; Cook, David C.; Hart, Terance W.; McLay, Iain M.; Jordan, Roy; Mason, Jonathan S.; Palfreyman, Malcolm N.; Walsh, Roger J. A.; et al.
 AUTHOR(S):
 CORPORATE SOURCE: Dagenham Res. Cent., Rhone-Poulenc Rorer, Dagenham/Essex, RM10 7XS, UK
 SOURCE: Journal of Medicinal Chemistry (1992), 35(20), 3613-24
 DOCUMENT TYPE: CODEN: JMCMAR; ISSN: 0022-2623
 LANGUAGE: English
 GI



AB The synthesis and biol. activity of trans-(.+-.)-N-methyl-2-(3-pyridyl)-2-tetrahydrothiopyrancarbothioamide 1-oxide (I), (RP 49356) and analogs is reported. Thus, I was prep'd. from 3-(chloromethyl)pyridine-HCl via oxidn. and cyclization of 4-chlorobutyl 3-pyridylmethyl sulfide to 2-(3-pyridyl)tetrahydrothiopyran 1-oxide. These compds. constitute a new structural class of K⁺-channel opener. The effects of changes in the pyridyl group, thioamide, and thiane ring on in vitro K⁺-channel opening activity are discussed. A 3-pyridyl or 3-quinolyl group, a small N-alkyl thioamide function, and a thiane oxide ring, in which the sulfoxide is in a trans relationship to the thioamide, are preferred for activity. Selected compds. were tested i.v. in the normotensive anesthetized rat for hypotensive effects, and the activities reflect their in vitro K⁺-channel opening activity. This led to further evaluation of compd. I and the selection of the (-)-enantiomer (RP 52891) for development as an antihypertensive and antianginal agent.

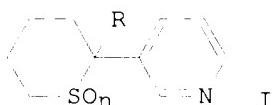
IT 143619-71-0P 143620-01-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. and amidation of)

RN 143619-71-0 CAPLUS
 RN 143620-01-3 CAPLUS

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L4 ANSWER 9 OF 17 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1991:535923 CAPLUS
 DOCUMENT NUMBER: 115:135923
 TITLE: Preparation of (1R,2R)-2-(3-pyridyl)tetrahydrothiopyran-2-thiocarboxamide-1-oxides
 INVENTOR(S): Aloup, Jean Claude; James, Claude; Margraff, Rodolphe
 PATENT ASSIGNEE(S): Rhone-Poulenc Sante, Fr.
 SOURCE: Eur. Pat. Appl., 14 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|-------------------|-----------------|----------|
| EP 426557 | A1 | 19910508 | EP 1990-403061 | 19901030 |
| EP 426557 | B1 | 19950222 | | |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE | | | | |
| FR 2653770 | A1 | 19910503 | FR 1989-14273 | 19891031 |
| FR 2653770 | B1 | 19920103 | | |
| AU 9065548 | A1 | 19910509 | AU 1990-65548 | 19901029 |
| AU 641950 | B2 | 19931007 | | |
| PL 164269 | B1 | 19940729 | PL 1990-287557 | 19901029 |
| IL 96160 | A1 | 19951231 | IL 1990-96160 | 19901029 |
| CA 2028985 | AA | 19910501 | CA 1990-2028985 | 19901030 |
| NO 9004708 | A | 19910502 | NO 1990-4708 | 19901030 |
| NO 177707 | B | 19950731 | | |
| NO 177707 | C | 19951108 | | |
| ZA 9008679 | A | 19910828 | ZA 1990-8679 | 19901030 |
| HU 59397 | A2 | 19920528 | HU 1990-6945 | 19901030 |
| HU 212501 | B | 19960729 | | |
| SU 1838311 | A3 | 19930830 | SU 1990-4831525 | 19901030 |
| ES 2068361 | T3 | 19950416 | ES 1990-403061 | 19901030 |
| JP 03153684 | A2 | 19910701 | JP 1990-292249 | 19901031 |
| US 5120852 | A | 19920609 | US 1990-607003 | 19901031 |
| PRIORITY APPLN. INFO.: | | FR 1989-14273 | | 19891031 |
| OTHER SOURCE(S): | | MARPAT 115:135923 | | |
| GI | | | | |



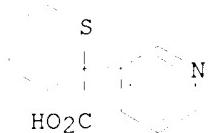
AB The title compds. [(1R,2R)-I; R = CSNHR1; R1 = Cl-4 alkyl; n = 1] (II) were prepnd. by oxidn. of I (R = H, n = 0) (III) and condensation of the product with R1NCS. Thus, (R,S)-III (prepn. given) was stirred 20 h at 20.degree. with cumyl hydroperoxide in aq. CH2Cl2 contg. di-Et (+)-tartrate and Ti(OCHMe2)4 to give, as 1 of 3 products, (1R,2R)-I (R = H, n = 1) which was stirred 10 min at -40 to -35.degree. with MeNCS in liq. NH3 contg. NaNH2 to give II (R1 = Me).

IT **86372-47-6**

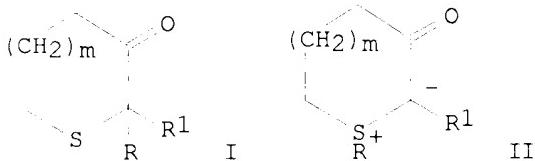
RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, in prepn. of pyridyltetrahydrothiopyranthiocarboxamide oxide)

09868894

RN 86372-47-6 CAPLUS
CN 2H-Thiopyran-2-carboxylic acid, tetrahydro-2-(3-pyridinyl)- (9CI) (CA INDEX NAME)

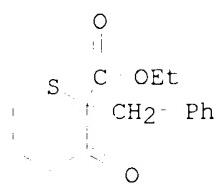


L4 ANSWER 10 OF 17 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1991:42500 CAPLUS
DOCUMENT NUMBER: 114:42500
TITLE: Rhodium carbenoid mediated cyclizations. Part 5.
Synthesis and rearrangement of cyclic sulfonium ylides; preparation of 6- and 7-membered sulfur heterocycles
AUTHOR(S): Moody, Christopher J.; Taylor, Roger J.
CORPORATE SOURCE: Dep. Chem., Imp. Coll. Sci., Technol. Med., London,
SW7 2AY, UK
SOURCE: Tetrahedron (1990), 46(18), 6501-24
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 114:42500
GI



AB The Rh₂(OAc)₄-catalyzed cyclization of 1,5- and 1,6-diazosulfides RS(CH₂)_nCOC(:N₂)R₁ (R = H, CH₂Ph, allyl, CH:CHCMe₂, (E)-CH₂CH:CHPh, R₁ = CO₂Et, COMe, n = 3, 4) gave thianes I (m = 1) and thiepanes I (m = 2) via cyclic sulfonium ylides II, which in some cases, e.g., II (R = CH₂PhEt, R₁ = CO₂Et, m = 1) could be isolated.
IT 120571-42-8P 120571-46-2P 120571-47-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 120571-42-8 CAPLUS
CN 2H-Thiopyran-2-carboxylic acid, tetrahydro-3-oxo-2-(phenylmethyl)-, ethyl ester (9CI) (CA INDEX NAME)

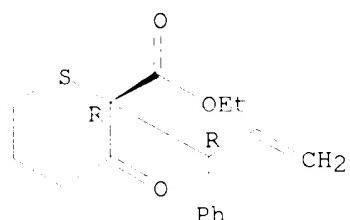
09868894



RN 120571-46-2 CAPLUS

CN 2H-Thiopyran-2-carboxylic acid, tetrahydro-3-oxo-2-(1-phenyl-2-propenyl)-, ethyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

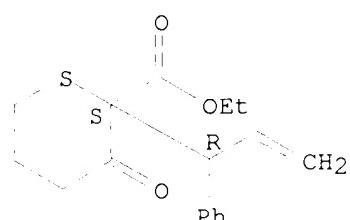
Relative stereochemistry.



RN 120571-47-3 CAPLUS

CN 2H-Thiopyran-2-carboxylic acid, tetrahydro-3-oxo-2-(1-phenyl-2-propenyl)-, ethyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 11 OF 17 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1989:496537 CAPLUS

DOCUMENT NUMBER: 111:96537

TITLE: Captodative substituent effects. 48. Spin delocalization in heterocyclic captodative radicals

AUTHOR(S): Nootens, C.; Merenyi, R.; Janousek, Z.; Viehe, H. G.
CORPORATE SOURCE: Lab. Org. Chem., Univ. Louvain, Louvain-la-Neuve,
1348, Belg.

SOURCE: Bull. Soc. Chim. Belg. (1988), 97(11-12), 1045-54

CODEN: BSCBAG; ISSN: 0037-9646

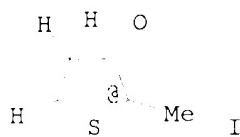
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 111:96537

GI

09868894



AB ESR of captodative radicals (e.g. I) are measured. Spin delocalization can be derived from different types of hyperfine coupling consts. Synthesis of radical precursors are described.

IT **122096-44-0P 122096-45-1P 122096-47-3P**

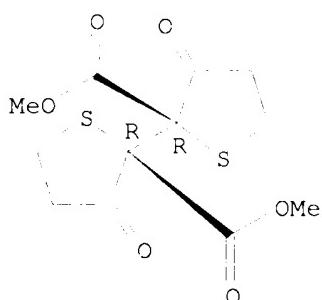
122096-52-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 122096-44-0 CAPLUS

CN [2,2'-Bithiophene]-2,2' (3H,3'H)-dicarboxylic acid, tetrahydro-3,3'-dioxo-, dimethyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

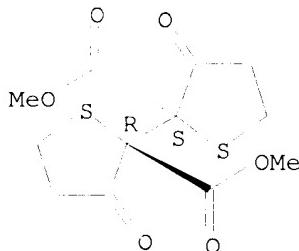
Relative stereochemistry.



RN 122096-45-1 CAPLUS

CN [2,2'-Bithiophene]-2,2' (3H,3'H)-dicarboxylic acid, tetrahydro-3,3'-dioxo-, dimethyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

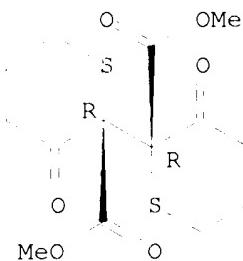


RN 122096-47-3 CAPLUS

CN [2,2'-Bi-2H-thiopyran]-2,2'-dicarboxylic acid, octahydro-3,3'-dioxo-, dimethyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

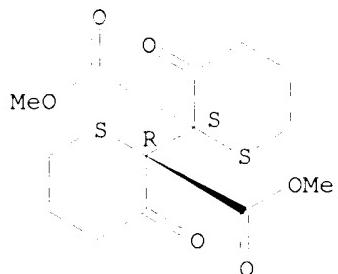
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RN 122096-52-0 CAPLUS

CN [2,2'-Bi-2H-thiopyran]-2,2'-dicarboxylic acid, octahydro-3,3'-dioxo-, dimethyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 12 OF 17 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1989:212554 CAPLUS

DOCUMENT NUMBER: 110:212554

TITLE: Rhodium carbenoid-mediated cyclizations. Synthesis and rearrangement of cyclic sulfonium ylides

Moody, Christopher J.; Taylor, Roger J.

CORPORATE SOURCE: Dep. Chem., Imperial Coll. Sci., Technol. + Med., London, SW7 2AY, UK

SOURCE: Tetrahedron Lett. (1988), 29(46), 6005-8

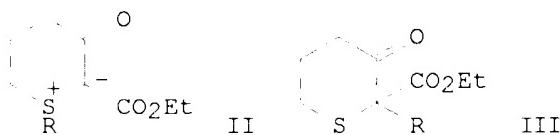
CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 110:212554

GI



AB Treatment of diazo sulfides with $\text{Rh}_2(\text{OAc})_4$ in C_6H_6 gives 6- and 7-membered cyclic sulfonium ylides; although S-benzyl and S-Et ylides can be isolated, they rearrange, or eliminate C_2H_4 , resp., on heating; the S-allyl ylides cannot be isolated since they undergo spontaneous [2,3]-sigmatropic rearrangement. Thus, decompn. of $\text{RS}(\text{CH}_2)_3\text{COC}(:\text{N}_2)\text{CO}_2\text{Et}$ (I; R = PhCH₂, Et) give cyclic ylides II, which rearrange to thiopyrans

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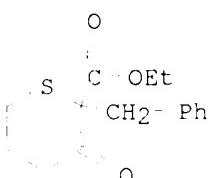
III ($R = PhCH_2$, H, resp.), upon heating. I ($R = allyl$), however, gives III ($R = allyl$) directly.

IT 120571-42-8P 120571-46-2P 120571-47-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 120571-42-8 CAPLUS

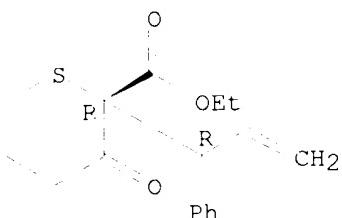
CN 2H-Thiopyran-2-carboxylic acid, tetrahydro-3-oxo-2-(phenylmethyl)-, ethyl ester (9CI) (CA INDEX NAME)



RN 120571-46-2 CAPLUS

CN 2H-Thiopyran-2-carboxylic acid, tetrahydro-3-oxo-2-(1-phenyl-2-propenyl)-, ethyl ester, (R^*, R^*)- (9CI) (CA INDEX NAME)

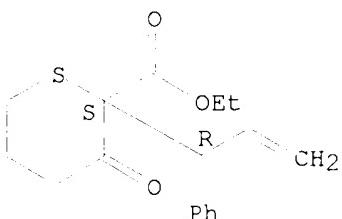
Relative stereochemistry.



RN 120571-47-3 CAPLUS

CN 2H-Thiopyran-2-carboxylic acid, tetrahydro-3-oxo-2-(1-phenyl-2-propenyl)-, ethyl ester, (R^*, S^*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 13 OF 17 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1988:549494 CAPLUS

DOCUMENT NUMBER: 109:149494

TITLE: A Wittig type rearrangement of 2-methoxycarbonyl-2-phenyl-1,3-dithiane and 2,2-diphenyl-1,3-dithiepane

AUTHOR(S): Inoue, Yoshihiko; Tanimoto, Shigeo

CORPORATE SOURCE: Inst. Chem. Res., Kyoto Univ., Uji, 611, Japan

SOURCE: Bull. Inst. Chem. Res., Kyoto Univ. (1987), 65(3), 121-4

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CODEN: BICRAS; ISSN: 0023-6071

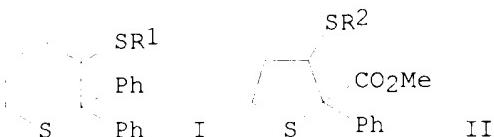
DOCUMENT TYPE:

Journal

LANGUAGE:

English

GI



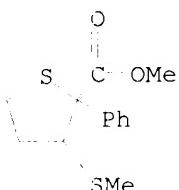
AB The title dithiepane was treated with LiN(CHMe₂)₂ and R₁I (R₁ = Me, Et) to give tetrahydrothiopyranyl sulfides I. Thiophanes II (R₂ = C₁₋₄ alkyl) were obtained from a disubstituted 1,3-dithiane deriv. and alkyl iodides and BuBr.

IT 116690-60-9P 116690-61-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

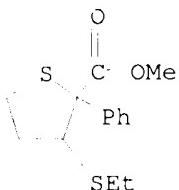
RN 116690-60-9 CAPLUS

CN 2-Thiophenecarboxylic acid, tetrahydro-3-(methylthio)-2-phenyl-, methyl ester (9CI) (CA INDEX NAME)



RN 116690-61-0 CAPLUS

CN 2-Thiophenecarboxylic acid, 3-(ethylthio)tetrahydro-2-phenyl-, methyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 14 OF 17 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1988:186601 CAPLUS

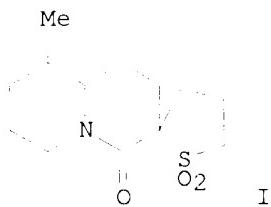
DOCUMENT NUMBER: 108:186601

TITLE: Spiro derivatives of tetrahydrothiophene. Phase transfer catalyzed alkylation of the 2-substituted tetrahydrothiophene system and the synthesis of spiro quinolizidine derivative

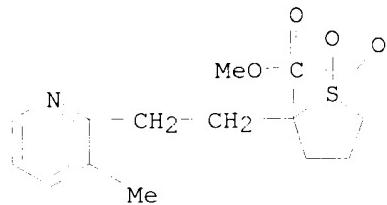
AUTHOR(S): Wrobel, Jerzy T.; Hejchman, Elzbieta

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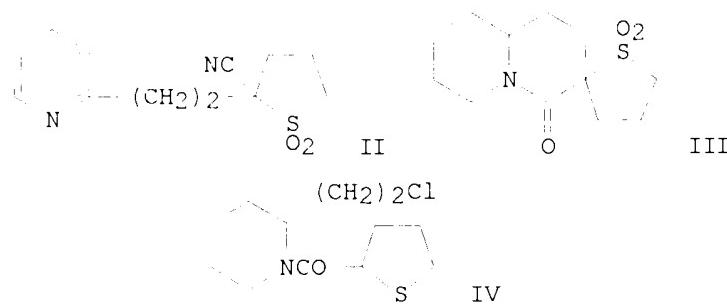
CORPORATE SOURCE: Chem. Dep., Warsaw Univ., Warsaw, 02-093, Pol.
SOURCE: Bull. Pol. Acad. Sci., Chem. (1987), 35(1-2), 21-9
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB The phase transfer catalyzed alkylation of 2-carbomethoxy- and 2-cyanotetrahydrothiophene, their sulfoxides, and sulfones is described. Key spiro deriv. I of quinolizidine was obtained from 2-(2-bromoethyl)-3-methylpyridine in three steps. Two stereoisomers of I were sep'd. and characterized.
IT **113990-96-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and cyclization cf)
RN 113990-96-8 CAPLUS
CN 2-Thiophenecarboxylic acid, tetrahydro-2-[2-(3-methyl-2-pyridinyl)ethyl]-, methyl ester, 1,1-dioxide (9CI) (CA INDEX NAME)



L4 ANSWER 15 OF 17 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1988:37629 CAPLUS
DOCUMENT NUMBER: 108:37629
TITLE: Spiro derivatives of tetrahydrothiophene. Synthesis
of the quinolizidine .ltbbrac.3-spiro-
2'.rtbbrac.tetrahydrothiophene system using
solid/liquid or liquid/liquid phase-transfer catalysis
AUTHOR(S): Wrobel, Jerzy T.; Hejchman, Elzbieta
CORPORATE SOURCE: Dep. Chem., Univ. Warsaw, Warsaw, PL-02-093, Pol.
SOURCE:
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 108:37629
GI



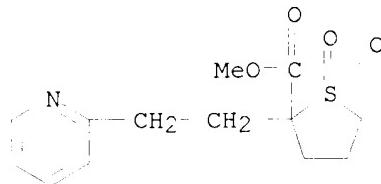
AB S-Cyanomethylation of Cl(CH₂)₃SH with ClCH₂CN gave 84% Cl(CH₂)₃SCH₂CN which was cyclized with aq. NaOH in the presence of PhCH₂NET₃+Cl⁻ to give 2-cyanotetrahydrothiophene (I) in 80% yield. Oxidn. of I with H₂O₂ in the presence of WO₃ gave its S, S-dioxide, which was deprotonated and alkylated with 2-(2-bromomethyl)pyridine to give II. Hydrolysis, esterification, hydrogenation, and cyclization gave the title spiro compd. III as a mixt. of stereoisomers. Hydrolysis of I, acid chloride formation, and condensation with 2-(2-chloroethyl)piperidine gave carboxamide IV. S-Oxidn. and cyclization under phase transfer conditions gave III as a single stereoisomer.

IT 112212-97-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn., hydrogenation, and cyclization of)

RN 112212-97-2 CAPLUS

CN 2-Thiophenecarboxylic acid, tetrahydro-2-[2-(2-pyridinyl)ethyl]-, methyl ester, 1,1-dioxide (9CI) (CA INDEX NAME)



L4 ANSWER 16 OF 17 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1983:453605 CAPLUS

DOCUMENT NUMBER: 99:53605

TITLE: Heterocyclic nitriles and their use for preparing medicines

INVENTOR(S): Aloup, Jean Claude; Bouchaudon, Jean; Farge, Daniel;
James, Claude

PATENT ASSIGNEE(S): Rhone-Poulenc Industries, Fr.

SOURCE: Fr. Demande, 25 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------|------|----------|-----------------|----------|
| FR 2511371 | A1 | 19830218 | FR 1981-15527 | 19810811 |

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| | | | | |
|---|----|----------|----------------|----------|
| FR 2511371 | B1 | 19840427 | | |
| EP 73704 | A1 | 19830309 | EP 1982-401501 | 19820806 |
| EP 73704 | B1 | 19861112 | | |
| R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE | | | | |
| AT 23530 | E | 19861115 | AT 1982-401501 | 19820806 |
| DK 8203594 | A | 19830212 | DK 1982-3594 | 19820810 |
| DK 158949 | B | 19900806 | | |
| DK 158949 | C | 19910311 | | |
| JP 58038281 | A2 | 19830305 | JP 1982-138063 | 19820810 |
| JP 03000394 | B4 | 19910107 | | |
| AU 8287022 | A1 | 19830512 | AU 1982-87022 | 19820810 |
| ZA 8205798 | A | 19830629 | ZA 1982-5798 | 19820810 |
| HU 30055 | O | 19840228 | HU 1982-2584 | 19820810 |
| HU 190029 | B | 19860828 | | |
| US 4456758 | A | 19840626 | US 1982-406998 | 19820810 |
| CA 1206149 | A1 | 19860617 | CA 1982-409078 | 19820810 |
| FI 8202801 | A | 19830212 | FI 1982-2801 | 19820811 |
| ES 514906 | A1 | 19830416 | ES 1982-514906 | 19820811 |
| PRIORITY APPN. INFO.: | | | FR 1981-15527 | 19810811 |
| | | | EP 1982-401501 | 19820806 |

OTHER SOURCE(S): CASREACT 99:53605

GI



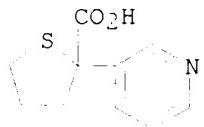
AB Nitriles I (X = O, S; X1 = S, CH₂, CH₂CH₂; R = cyano; R¹ = N heterocyclic) were prep'd. as intermediates for antihypertensive (no data) I (R = thiocarbamoyl). Thus 3-pyridylacetonitrile was treated with Br(CH₂)₃SCN to give I (X = S, X1 = CH₂, R = cyano, R¹ = 3-pyridyl) which was hydrolyzed to the acid, converted to the acid chloride, amidated with MeNH₂, and thiolated with Lawesson's reagent to give I (X = S, X1 = CH₂, R = CSNHMe, R¹ = 3-pyridyl).

IT **86372-40-9P 86372-47-6P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prep'n. and chlorination of)

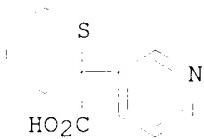
RN 86372-40-9 CAPLUS

CN 2-Thiophenecarboxylic acid, tetrahydro-2-(3-pyridinyl)- (9CI) (CA INDEX NAME)



RN 86372-47-6 CAPLUS

CN 2H-Thiopyran-2-carboxylic acid, tetrahydro-2-(3-pyridinyl)- (9CI) (CA INDEX NAME)



L4 ANSWER 17 OF 17 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1968:428568 CAPLUS
 DOCUMENT NUMBER: 69:28568
 TITLE: Theoretical and spectroscopic studies of indigo dyes.
 VII. Preparation of 3,3'-dioxo-4,4,4',4'-tetramethyl-
 2,2'-bithiolanylidene, a compound with the basic
 chromophore system of thioindigo dyes
 AUTHOR(S): Hermann, Heinrich; Luettke, Wolfgang
 CORPORATE SOURCE: Univ. Goettingen, Goettingen, Ger.
 SOURCE: Chem. Ber. (1968), 101(5), 1708-14
 CODEN: CHBEAM
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 GI For diagram(s), see printed CA Issue.
 AB The treatment of ClCOCH₂SCH₂CMe₂COCl with tert-BuOH in pyridine gave
 4,4-dimethyl-2-tert-butoxycarbonylthiolan-3-one (I, R = CO₂CMe₃), which
 reacted with K₃Fe(CN)₆ in CF₃CO₂H to give 3,3'-dioxo-4,4,4',4'-tetramethyl-
 trans-2,2'-bithiolanylidene (II) via 3,3'-dioxo-4,4,4',4'-tetramethyl-2,2'-
 bis-tert-butoxycarbonyl-2,2'-bithiolanyl and 3,3'-dioxo-4,4,4',4'-
 tetramethyl-2,2'-bithiolanyl. II was also prep'd. by the
 dehydrodimerization of I (R = H).
 IT 20048-22-OP
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 20048-22-0 CAPLUS
 CN [2,2'-Bithiophene]-2,2'(3H,3'H)-dicarboxylic acid, tetrahydro-4,4,4',4'-
 tetramethyl-3,3'-dioxo-, di-tert-butyl ester (8CI) (CA INDEX NAME)

